Numerical simulation of hydrogen transport and accumulation in multilayer metal membranes under damaging neutron irradiation [[1]](#footnote-1)\*)

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This work describes the development of the computational code [1] for simulation the effect of radiation damage to metals (such as formation of radiation vacancies) on the kinetic characteristics of hydrogen - the effective diffusion coefficient, the flow through the wall of the vacuum chamber and its accumulation in the material for thermonuclear and hybrid (fusion-fission) reactors based on tokamak [2]. The model was supplemented to include the isotope effect, the presence of dislocations and grain boundaries in a metal membrane, and the boundaries between materials in the case of multilayer metal membranes. A calculation was made of the permeating flux of hydrogen (for various isotopes) and its accumulation in structural and plasma-facing materials under conditions characteristic of thermonuclear and hybrid (fusion-fission) tokamak reactors. At the current stage, approximations were used to simulate materials and their combinations: chromium-zirconium bronze was modeled with pure copper, steels were modeled by the bcc iron phase. Tungsten, which is a candidate material for plasma-facing elements, was also modeled.

This work demonstrates that different hydrogen isotopes are equally confined by traps in a metal in the case of a harmonic approximation for determining the diffusion coefficients of isotopes. In Fe, in the temperature range T <600 K, a strong increasing of trapped hydrogen concentration is observed, and at T <350 K it exceeds the concentration of free hydrogen. This feature is explained by the accumulation of vacancies under the action of damaging neutron irradiation at low temperatures, as well as by a decrease in the ability of hydrogen to leave the trap due to the low temperature. In the region T> 1100K in W, the concentration of held hydrogen is 6–7 orders lower than the concentration of free hydrogen, which is explained by the high energy of vacancy formation in W, compared to Fe and Cu, and also by the active process of dissociation of complexes of the "vacancy-hydrogen atom" type. In the intermediate temperature range T ∈ [1000K, 1100K], a noticeable increase in the concentration of retained hydrogen is observed in Cu compared to W. In this layer, up to 1% of hydrogen is in a state bound to vacancies. This increase in the concentration of held hydrogen is due to the low energy of vacancy formation in copper (which creates a large number of traps for hydrogen in the presence of damaging neutron irradiation), as well as the relatively high binding energy of the vacancy-hydrogen atom complexes.

Estimates of the permeation fluxes of hydrogen through various in-chamber elements of the facility were obtained, as well as the accumulation of hydrogen isotopes in them for the conditions of the DEMO-TIN facility [2].

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References

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1. \*) [abstracts of this report in Russian](http://www.fpl.gpi.ru/Zvenigorod/XLVIII/Mu/ru/AO-Suslin.docx) [↑](#footnote-ref-1)